

ADVECTION OF METHANE IN THE HYDRATE ZONE: MODEL, ANALYSIS AND EXAMPLES

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ABSTRACT. A two-phase two-component model is formulated for the advective-diffusive transport of methane in liquid phase through sediment with the accompanying formation and dissolution of methane hydrate. This free-boundary problem has a unique generalized solution in L^1 ; the proof combines analysis of the stationary semilinear elliptic Dirichlet problem with the non-linear semigroup theory in Banach space for an m -accretive multi-valued operator. Additional estimates of maximum principle type are obtained, and these permit appropriate maximal extensions of the phase-change relations. An example with pure advection indicates the limitations of these estimates and of the model developed here. We also consider and analyze the coupled pressure equation that determines the advective flux in the transport model.

1. INTRODUCTION

Methane hydrates are crystalline solid compounds consisting of methane molecules encased in a cage of water molecules. These solids are stable only at the combined low temperatures and high pressures found in offshore continental slopes or permafrost regions. Methane hydrates have been a subject of intense geophysics research for decades due to their potential as energy sources or as hazards to climate or seafloor stability [1, 2, 3, 4]. The modeling of methane hydrate formation and stability requires the use of multi-phase flow models to quantify the exchange of components between phases in combination with a thermodynamically consistent description of the dynamic partitioning of these components [5, 6, 7, 8]. Moreover, the occurrence of hydrates is tied to the availability and type of advective pathways and the associated permeability and porosity of the host medium [9, 10, 11, 12, 13]. The mathematical difficulties presented by any realistic model include systems of partial differential equations with degeneracy and multi-valued representations of phase change.

In [14] we took a first step towards the analysis of well-posedness of a simplified methane hydrate system. We assumed geothermal and hydrostatic equilibrium, and thus no energy or pressure equations were necessary. We considered diffusion as the only transport mechanism, and represented the phase change using variational inequalities or nonlinear complementarity constraints which vary with depth. The theory developed in [14] gives a time-differentiable solution for which the evolution equation holds in a space of distributions, H^{-1} , but the methods apply only to self-adjoint (diffusive) form of transport. Furthermore, we defined a fully implicit in time finite element scheme for the problem and demonstrated that it converges at the same rate as a similar scheme for Stefan free-boundary problem.

The system formulated and analyzed in this paper accounts for the transport of methane by means of both fluid advection and diffusion, and for the coupled pressure equation which gives advective flux. It is motivated by observations of massive hydrate deposits which could not have occurred by diffusion only. Rather, a combination of advective flux together with local biogenic

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production of methane is required for the accumulation of such massive deposits over realistic time scales [15, 9]. The necessity to include advection motivated us to go beyond the earlier results of [14] and obtain additional estimates on the components of the solution. In this paper we shall obtain a solution which is continuous with values in the function space L^1 ; although smoother in the spatial variable, it is formally less smooth in time. Furthermore, in this paper we account for the pressure equation which is coupled to the methane transport model and can be formulated in several variants. To model the coupled transport-pressure system we use a staggered-in-time strategy.

This paper is organized as follows. In Section 2 we introduce some mathematical concepts and notation that will be used thereafter. In Section 3 we describe the transport model which, as in [14], is of compositional flow type with two phases, solid and liquid, and two components, water and methane. Additionally we describe the pressure equation coupled to the transport model, which is not covered in [14]. After some simplifications, the transport model is a partial differential equation whose solution is subject to constraints which vary with the depth. These constraints appear as complementarity conditions or as variational inequalities on the solution. In addition, we describe variants of the pressure equation coupled to the model.

The simplified transport model is proven in Section 4 to be well-posed and to satisfy a useful estimate of maximum principle type. These results apply to a general class of semilinear elliptic-parabolic partial differential equations in which the nonlinearity may depend on the spatial variable. Section 5 contains an explicit 1D example (without diffusion) which indicates some limitations of the model by means of the blow-up that results from non-homogeneous boundary flux conditions or large initial data. In Section 6 we discuss the time-dependent system with the transport model coupled to the pressure equation, whose solution and analysis relies on a loosely coupled staggered in time scheme. Section 7 contains possible extensions of this work and some work underway.

2. NOTATION AND PRELIMINARIES

Here we introduce some notation and recall the theory that will be used in the following. First, we denote the extended real number system by $\mathbb{R}_\infty \equiv (-\infty, +\infty]$. An extended real-valued function $\varphi : \mathbb{R} \rightarrow \mathbb{R}_\infty$ is *convex* if

$$(1) \quad \varphi(tu + (1-t)v) \leq t\varphi(u) + (1-t)\varphi(v) \text{ for } u, v \in \mathbb{R}, \ 0 \leq t \leq 1.$$

It is *proper* if $\varphi(\xi) < \infty$ for some $\xi \in \mathbb{R}$ and its *effective domain* is the set $\text{Dom}(\varphi) = \{\xi \in \mathbb{R} : \varphi(\xi) < \infty\}$. For such a function, the *subgradient* of φ at $u \in \text{Dom}(\varphi)$ is the set of all $u^* \in \mathbb{R}$ such that

$$u^*(v - u) \leq \varphi(v) - \varphi(u) \text{ for all } v \in \mathbb{R},$$

and this set is denoted by $\partial\varphi(u)$. The *maximal monotone* graphs in $\mathbb{R} \times \mathbb{R}$ are characterized as the subgradients of proper convex lower-semicontinuous functions on \mathbb{R} . These multi-valued relations extend the notion of a continuous monotone function. Related results hold in any Hilbert space, but we shall not need that generality here [16, 17, 18, 19, 20].

As an example, we consider the set of pairs x, y that are related by

$$y \leq 0, \ x \geq 0, \ yx = 0.$$

This arises in the *complementarity problem*, a special *variational inequality*, where $y = f - A(x)$ when f and the function $A(\cdot)$ are given [21, 22, 23]. If we let $I^+(\cdot)$ be the *indicator function* of the positive real numbers, that is, $I^+(x) = 0$ if $x \geq 0$ and $I^+(x) = +\infty$ if $x < 0$, then $I^+(\cdot)$ is a proper, convex and lower-semicontinuous function, and the complementarity conditions are equivalent to

$$y(z - x) \leq I^+(z) - I^+(x) \text{ for all } z \in \mathbb{R}.$$

This is the *subgradient* constraint $y \in \partial I^+(x)$ which characterizes the maximal monotone relation $\partial I^+(\cdot)$ on $\mathbb{R} \times \mathbb{R}$. It is approximated by the derivative $y = \frac{d}{dx} I_\lambda^+(x)$ of the regularized indicator function,

$$I_\lambda^+(x) = \begin{cases} 0 & \text{if } x \geq 0, \\ \frac{x^2}{2\lambda} & \text{if } x < 0, \end{cases} \quad \text{for which} \quad \frac{d}{dx} I_\lambda^+(x) = \begin{cases} 0 & \text{if } x \geq 0, \\ \frac{x}{\lambda} & \text{if } x < 0. \end{cases}$$

This special case will be used below.

We shall use below the *positive part* function, $x^+ = \frac{1}{2}(x + |x|)$, the signum graph, $\text{sgn}(x) = \{\frac{x}{|x|}\}$ for $x \neq 0$ and $\text{sgn}(0) = [-1, 1]$, and the subgradient of x^+ , namely, $\text{sgn}^+ = \frac{1}{2}(1 + \text{sgn}(x))$. We denote by sgn_0 the corresponding (single-valued) function with $\text{sgn}_0(0) = 0$ and similarly with sgn_0^+ . Finally, we denote the gradient of a function $p(\cdot)$ by the (column) vector of partial derivatives, $\nabla p = (\partial_1 p, \dots, \partial_N p)^T$ and the divergence of the vector function $\mathbf{q}(\cdot) = (q_1, \dots, q_N)^T$ by $\nabla \cdot \mathbf{q} = \sum_{j=1}^N \partial_j q_j$.

Measurable-convex integrands. Let G be an open bounded domain in \mathbb{R}^N . Assume that the extended-real-valued function $\varphi(x, \xi)$ is a *measurable-convex integrand*:

- for each $x \in G$, the function $\varphi(x, \cdot) : \mathbb{R} \rightarrow \mathbb{R}_\infty$ is proper, lower-semicontinuous and convex, and
- for each $\xi \in \mathbb{R}$, the function $x \mapsto \varphi(x, \xi)$ is measurable.

This notion was developed in [18, 19] and applied in [14].

A useful regularization of such functions is the *Moreau-Yosida approximation*: for $\lambda > 0$, set

$$(2) \quad \varphi_\lambda(x, r) = \inf_{t \in \mathbb{R}} \left\{ \frac{1}{2\lambda} |r - t|^2 + \varphi(x, t) \right\}.$$

Each of these has a derivative,

$$\beta_\lambda(x, r) = \frac{\partial}{\partial r} \varphi_\lambda(x, r), \quad r \in \mathbb{R},$$

which is Lipschitz continuous on \mathbb{R} with constant $1/\lambda$, and we have monotone convergence

$$\lim_{\lambda \rightarrow 0^+} \varphi_\lambda(x, r) = \varphi(x, r), \quad x \in G.$$

For each $x \in G$, we denote the subgradient of $\varphi(x, \cdot)$ by $\beta(x, \cdot) = \partial \varphi(x, \cdot)$. Such a family of maximal monotone graphs will be used to formulate our problem.

Accretive operators and initial-value problems.

Definition 2.1. An operator (relation) \mathbb{A} on a Banach space X is accretive if for $[x_j, y_j] \in \mathbb{A}$, $j = 1, 2$ and $\lambda > 0$, we have

$$\|x_1 - x_2\| \leq \|(x_1 + \lambda y_1) - (x_2 + \lambda y_2)\|.$$

This is equivalent to requiring that $(I + \lambda \mathbb{A})^{-1}$ is a contraction on $Rg(I + \lambda \mathbb{A})$ for each $\lambda > 0$. An accretive operator \mathbb{A} is m-accretive on X if additionally the range condition $Rg(I + \lambda \mathbb{A}) = X$ holds for every $\lambda > 0$.

Consider now an m-accretive operator \mathbb{A} and an evolution equation

$$(3) \quad u'(t) + \mathbb{A}u(t) \ni F(t), \quad 0 < t < T, \quad u(0) = u_0.$$

The nonlinear semigroup generation theorem asserts that if \mathbb{A} is an m-accretive operator on the Banach space X , the Cauchy problem (3) is well-posed [24, 25, 20]. It gives a solution which is minimally smooth in time.

Definition 2.2. An ε -solution of (3) is a discretization

$$(4) \quad \mathcal{D} \equiv \{0 = t_0 < t_1 < \dots < t_N = T; F_1, \dots, F_N \in X\}$$

and a step function

$$(5) \quad s(t) \equiv \begin{cases} s_0 & t = t_0 \\ s_j & t \in (t_{j-1}, t_j] \end{cases}$$

for which

$$\begin{aligned} t_j - t_{j-1} &\leq \varepsilon \text{ for } 1 \leq j \leq N, \\ \sum_{j=1}^N \int_{t_{j-1}}^{t_j} \|F(t) - F_j\| dt &< \varepsilon, \text{ and} \\ \frac{s_j - s_{j-1}}{t_j - t_{j-1}} + \mathbb{A}(s_j) &\ni F_j, \quad 1 \leq j \leq N. \end{aligned}$$

The step function (5) provides a natural approximate solution to (3) by backward differences in time.

Definition 2.3. A C^0 -solution to (3) is a function $u \in C([a, b]; X)$ such that for each $\varepsilon > 0$ there is an ε -solution \mathcal{D}, s of (3) with

$$\|u(t) - s(t)\| \leq \varepsilon.$$

The nonlinear semigroup theory [20, p.228] shows that the Cauchy problem (3) is well-posed with this notion of solution.

Theorem 2.4. Let \mathbb{A} be m -accretive on a Banach space X . For each $u_0 \in \overline{\text{Dom}(\mathbb{A})}$ and $F \in L^1(0, T; X)$ there is a unique C^0 -solution of the Cauchy problem (3).

See [26, 27, 28, 24, 25, 29, 30, 31, 32] for development and applications of this theory to problems of structure similar to that considered in this paper.

The objective in Section 4 is to transform the hydrate transport model developed in Section 3 into a form to which Theorem 2.4 can be applied.

3. THE MODEL

In this Section we describe the model for methane transport as well as the coupled pressure equation.

The subseafloor region $G \subset \mathbb{R}^3$ is a porous sediment of porosity ϕ and permeability κ through which the liquid phase (brine) can flow. This liquid phase may have some methane gas dissolved in it; the methane component is supplied by microbial activity, or is supplied from much deeper earth layers. If the amount of methane attains a certain maximum amount for a given pressure and temperature, methane comes out of the liquid solution in form of either free gas or methane hydrate, and that form depends on the pressure and temperature conditions. Methane hydrate, an ice-like substance, forms in conditions of high pressure $p(x, t)$ and low temperature $T(x)$, while free gas forms at higher temperatures or lower pressures, or if there is not enough water available. It is the formation of the hydrate and its possible dissociation in the hydrate zone with abundance of water component that we wish to describe in this paper. Inclusion of a free gas phase in the model is the subject of ongoing work and will not be discussed here.

The phases within the pore system are *liquid* and *hydrate* indexed by subscripts $i = \ell, h$. *Phase saturation* is the volume fraction $S_i(x, t)$ of phase i present in the pores. Assume there is no (free) gas phase present here, so these two phases fill the pore space: $S_\ell + S_h = 1$. The components are *water* and *methane* indexed by superscripts $j = W, M$. The *density* of phase i

is $\rho_i = \rho_i^W + \rho_i^M$, $i = \ell, h$, where ρ_i^j is the *mass concentration* of component j in phase i . The corresponding *mass fractions* are $\chi_i^M = \frac{1}{\rho_i} \rho_i^M$, $\chi_i^W = \frac{1}{\rho_i} \rho_i^W$, $i = \ell, h$, so we have $0 \leq \chi_i^j \leq 1$ and $\chi_i^M + \chi_i^W = 1$. Also we assume abundant water component $\chi_\ell^W > 0$.

3.1. Transport model with phase constraints. The *mass conservation* equation for the methane component takes the form

$$(6) \quad \frac{\partial}{\partial t}(\phi S_\ell \rho_\ell \chi_\ell^M + \phi S_h \rho_h \chi_h^M) + \nabla \cdot \mathbf{J}_\ell^M = f_M$$

in which the flux of the methane in the liquid has an advective and a diffusive part

$$(7) \quad \mathbf{J}_\ell^M = \rho_\ell \chi_\ell^M \mathbf{q} - \rho_\ell D_\ell^M \nabla \chi_\ell^M.$$

The flux \mathbf{q} is the *Darcy velocity*. The molecular diffusion term $-\rho_\ell D_\ell^M \nabla \chi_\ell^M$ arises from Fick's law, and the diffusivity D_ℓ^M can be scaled as in [33, 2.2-20] with porosity and liquid saturation, but will be simplified here by assuming $D_\ell^M \equiv \text{const}$ as is done in [9, 14].

State Equations. Additional conditions that are special to the situation studied here include the following. The liquid is *incompressible*: $\rho_\ell = \text{constant}$. We also assume that water phase is present everywhere, so $S_\ell > 0$ and liquid pressure $p(x, t)$ is defined everywhere. *Salt* content of the brine (liquid phase) χ_l^S and *temperature* $T(x)$ are assumed to be known and constant in time. The temperature $T(x)$ is assumed to be linearly increasing with depth, and $\chi_l^S \equiv \text{const}$ is assumed to be that of seawater. The content of the hydrate phase is fixed, so its properties ρ_h^W , ρ_h , ρ_h^M , χ_h^W , χ_h^M are all known constants. Finally, we mention the need as in [9] to distinguish between different rock types of a given sediment by assigning to it a categorical variable $r(x)$.

The remaining χ_ℓ^M and $S_h = 1 - S_\ell$ are essential unknowns.

Phase Equilibria. Let

$$\chi^*(p(x, t), T(x), \chi_l^S(x, t), r(x))$$

denote the *maximal mass fraction* of methane that can be dissolved in the liquid for the given pressure p , temperature T , and salinity χ_l^S in sediment of rock type $r(x)$. Typically χ^* increases with temperature (thus with depth), has only mild dependence on $p(x, t)$ and $\chi_l^S(x)$, but can vary substantially between different rock types [9]. (Dependence of χ^* on $p(x, t)$ is strong in the gas zone which is not considered here). Assuming these are known, we see that the methane *maximum solubility constraint* χ^* can be approximated as a function of x

$$(8) \quad \chi^*(p(x, t), T(x), \chi_l^S(x, t), r(x)) \approx \chi^*(x).$$

Now the hydrate is present only where the liquid is fully saturated, so $\chi_\ell^M = \chi^*(x)$ in the hydrate region. That is, the dissolved mass fraction takes the *maximal* value wherever $S_h > 0$: $S_h > 0$ implies $\chi_\ell^M = \chi^*(x)$. Conversely, if the amount of methane does not attain $\chi^*(x)$, then no hydrate can be present: $\chi_\ell^M < \chi^*(x)$ implies $S_h = 0$. In summary, the hydrate saturation and liquid mass fraction of methane satisfy the *complementarity constraints* [34]

$$(9) \quad \begin{cases} S_h \geq 0, \\ \chi^*(x) - \chi_\ell^M \geq 0, \\ S_h (\chi^*(x) - \chi_\ell^M) = 0. \end{cases}$$

To make the model physically meaningful, we need to have

$$(10) \quad S_h \leq 1, \quad \chi_l^M \geq 0.$$

Ensuring (10) is the crux of the analysis presented in Section 4 and, as we show, is not always possible. Since solutions violating (10) are unphysical, the question arises of whether the model is therefore adequate, or whether the analysis is lacking. These issues are addressed in Section 7.

The Transport Equation. Now we introduce the choice of variables S, χ , functions of the point $x \in G$ and time $t > 0$:

$$S \equiv S_h(x, t) = 1 - S_\ell(x, t), \quad \chi \equiv \chi_\ell^M(x, t).$$

After division by ρ_ℓ , the mass conservation equation for methane (6) is

$$(11a) \quad \frac{\partial}{\partial t}(\phi(1 - S)\chi + \phi S R) + \nabla \cdot (\mathbf{q}\chi - D_\ell^M \nabla \chi) = \frac{1}{\rho_\ell} f_M$$

with two unknowns χ and S , and where we have set

$$(11b) \quad R := \frac{\rho_h \chi_h^M}{\rho_\ell}.$$

We can also define for future convenience the (dimensionless) total methane content per mass of liquid phase

$$(11c) \quad u := \phi(1 - S)\chi + \phi S R.$$

The two variables χ and S are connected by the phase equilibrium condition (9) written as a subgradient,

$$(11d) \quad \chi \in \chi^*(x, p) + \partial I^+(S),$$

where $I^+(\cdot)$ denotes the indicator function of the positive real numbers. For simplicity, we shall assume

$$(12) \quad \phi(x, t) = 1, \quad x \in G,$$

but we confirm in Remark 4.5 that this assumption is unnecessary.

Since S is a monotone relation in χ , and since as is known in practice [6, 14],

$$(13) \quad \chi \leq \chi^*(x) < R,$$

the system (11) is a semi-linear *porous medium equation* [35]

$$(14) \quad \frac{\partial}{\partial t} \beta(x, \chi) + \nabla \cdot (\mathbf{q}\chi - D_\ell^M \nabla \chi) \ni f, \quad x \in G, \quad 0 < t < T,$$

with advection and an x -dependent family of multi-valued monotone graphs $\beta(x, \cdot)$. The equation (14) is similar to the *Stefan problem*, but with advection and with x -dependence of the constraints. In the Stefan problem the variable u would play the role of enthalpy, and χ would be temperature. The model (11) occurs as equation (3) in [9], and as part of the comprehensive models developed in [6] where $p(x, t), T(x, t), \chi_\ell^S(x, t)$ vary and are unknowns.

The advection-free case of (11) in \mathbb{R}^N with $\mathbf{q} = \mathbf{0}$ was analyzed in [14] in the Hilbert space $H^{-1}(G)$, but the analysis there depended on the symmetry of the linear elliptic operator $-\nabla \cdot D_\ell^M \nabla$ and does not extend to the case $\mathbf{q} \neq \mathbf{0}$. The results of [36] formally may apply to give existence of a solution of (11) in $H^{-1}(G)$ when the elliptic part of (11) is coercive, and uniqueness if additionally $\mathbf{q} = \mathbf{0}$. However, since the maximum estimate is not available for these solutions, they have limited interest here.

The objectives in Section 4 are to analyze the initial-boundary-value problem for the advection-diffusion system (14) together with a maximum principle. In particular, by (11c), the constraints (10) are equivalent to

$$(15) \quad 0 \leq u(x, t) \leq R,$$

and deriving estimates on the solution so that the physically meaningful bound (15) holds, is a challenge addressed in Section 4. In order to apply these abstract results to (14), we shall need to extend the relations $\beta(x, \cdot)$ to a family of maximal monotone graphs $\bar{\beta}(x, \cdot)$, and the estimates

obtained below will in some cases assure that our solution satisfies (15) and so is independent of these extensions. Other cases require a more general modeling framework in which the pressure equation is an important component.

3.2. The Pressure Equation. The *pressure* $p(x, t)$ and *Darcy velocity* $\mathbf{q}(x, t)$ of the filtrating liquid are derived by summing mass conservation equations for all components as in ([33], Chapter 2). Since χ_l^S is assumed constant, in our case this would be summing (6) plus an equation for χ_l^W . This leads to a simplified version of the pressure equation in which we drop diffusion terms,

$$(16) \quad \frac{\partial}{\partial t}(\phi(\rho_l S_l + S_h \rho_h)) + \nabla \cdot (\rho_l \mathbf{q}) = 0.$$

Further simplifying and assuming $\phi \approx \text{const}$, $\rho_l \approx \rho_h$ as well as incompressibility gives

$$(17a) \quad \nabla \cdot \mathbf{q} = 0,$$

The problem is closed with Darcy's law

$$(17b) \quad \frac{\mu}{\kappa} \mathbf{q} = -(\nabla p - \rho_l \mathbf{g}),$$

where $\mathbf{g} = -\mathbf{e}_3 g$ is the gravity vector.

Superficially, it appears that the coupling between the transport equation (6) and the Darcy flow (17) is one way only in this model due to the simplified form of the pressure equation and due to (8). A more comprehensive version of pressure equation such as (16) would yield two-way coupling, and may involve further nonlinearities if, e.g., the dependence of porosity ϕ on the pressure is known, or is modeled by geomechanics coupling.

More generally, the porosity or permeability may vary with time due to the deposition of hydrate, $\phi(x, t) = \phi(p(x, t))$ and $\kappa(x, t) = \kappa(x, S(x, t))$ in the pressure equation (17b), and the liquid pressure p and Darcy velocity \mathbf{q} are likewise time-dependent. This general case may also be included in the more general evolution pressure equation (16).

Hydrostatic pressure and excess pressure. In [14, 7] we assumed that pressure is hydrostatic, that is, that the right side of (17b) vanishes and, consequently, pressure increases linearly with depth according to hydrostatic gradient, and $\mathbf{q} = \mathbf{0}$. In order to account for nonzero flux \mathbf{q} , we solve (17), but decompose $p(x, t)$ further into its hydrostatic part $p^0(x)$ and excess pressure $p^*(x, t)$.

The *hydrostatic pressure* $p^0(x)$ is determined by depth

$$(18a) \quad \mathbf{q}^0 = \mathbf{0},$$

$$(18b) \quad \nabla p^0 = \rho_l \mathbf{g}.$$

Then the *excess pressure* $p^*(x, t)$ associated with \mathbf{q} satisfies

$$(19a) \quad \nabla \cdot \mathbf{q} = 0,$$

$$(19b) \quad \mu \kappa^{-1} \mathbf{q} = -\nabla p^*.$$

The flux $\mathbf{q}(x, t)$ is determined by either the total pressure from (17) or the excess pressure from (19). This decomposition is useful in numerical approximation.

In particular, for a slightly compressible medium, a pressure-porosity relation $\phi(x, t) = \Phi^*(x, p^*(x, t))$ is determined by the local mechanics of the medium, but

$$(20) \quad \kappa = \kappa(S)$$

is, in general, not known exactly (see [6] for some algebraic approximate formulas). In fact, (20) may be extended by pressure-stress dependence as well.

4. ANALYSIS OF TRANSPORT MODEL

In this section we shall obtain existence-uniqueness of an L^1 -solution and maximum estimates for an initial-value problem for the semilinear equation (14) with (homogeneous) Dirichlet boundary conditions. These results are obtained for a problem in which the graphs $\beta(x, \cdot)$ have been extended to maximal monotone graphs $\bar{\beta}(x, \cdot)$ which agree with $\beta(x, \cdot)$ on the set of interest.

The general plan is to apply Theorem 2.4 to an abstract version of (14). To do so, in Section 4.1 we make precise the elliptic operator A_1 needed in (14) and its properties on $L^1(G)$. Next we construct the operator $\mathbb{A} = A \circ \bar{\beta}^{-1}(x, \cdot)$ from a general operator A of which the elliptic operator A_1 is an example. Here $\bar{\beta}$ has to be maximal monotone, and for our application it is x -dependent. We handle the x -dependent case by the methods of [37] and in Section 4.2 we supplement these results to resolve the stationary problem that results from a backward-difference approximation of (14), namely,

$$(21) \quad \bar{\beta}(x, v(x)) + Av(x) \ni f(x).$$

These results show that \mathbb{A} is m-accretive, and we describe comparison and maximum estimates for the stationary problem. In Section 4.3 we put together the properties of \mathbb{A} and the abstract nonlinear semigroup theory from Section 2 to conclude well-posedness of (14) with the extension $\bar{\beta}$ of β . Related estimates are formulated for the evolution problem.

The use of $\bar{\beta}(x, \cdot)$ in (14) instead of $\beta(x, \cdot)$, which is not maximal, requires some a-priori assumptions on the solution. The comparison and maximum principles show where such a-priori conditions can be eliminated, as they are consequences of the data. The final result of this Section is Proposition 4.9 which applies the abstract results to obtain well-posedness of (14). In Section 5 we provide explicit examples where the a-priori conditions can and cannot be eliminated.

4.1. Elliptic operator A_1 and its properties. Define the usual continuous bilinear form on the Sobolev space $V = H_0^1(G)$ corresponding to an advection-diffusion-reaction problem

$$(22) \quad \mathcal{A}v(\psi) = \sum_{i,j=1}^N \int_G a_{ij}(x) \partial_i v \partial_j \psi \, dx - \sum_{j=1}^N \int_G q_j(x) v \partial_j \psi \, dx + \int_G a(x) v \psi \, dx, \quad v, \psi \in V.$$

Assume the coefficients a_{ij} , $q_j \in C^1(\bar{G})$, $a \in L^\infty(G)$ satisfy

$$(23) \quad a(x) \geq 0, \quad 2a(x) + \partial_j q_j \geq 0, \quad a_{ij}(x) \xi_i \xi_j \geq c_0 |\xi|^2, \quad x \in G, \quad \xi \in \mathbb{R}^N.$$

Remark 4.1. In (14) we have $a \equiv 0$, $\nabla \cdot \mathbf{q} = 0$, and $a_{ij} = D_i^M \delta_{ij}$ hence (23) holds.

Now define

$$(24) \quad A_1 v = - \sum_{i,j=1}^N \partial_j (a_{ij} \partial_i v) + \sum_{j=1}^N \partial_j (q_j v) + av.$$

with $\text{Dom}(A_1) \equiv \{v \in W_0^{1,1}(G) : A_1 v \in L^1(G)\}$ where $A_1 v = f \in L^1(G)$ corresponds to the Dirichlet problem

$$v \in W_0^{1,1}(G) : \mathcal{A}v(\psi) = \int_G f \psi \, dx, \quad \psi \in C_0^\infty(G).$$

Note that (22) is well defined for $(v, \psi) \in (W_0^{1,1}(G), C_0^\infty(G))$ and determines $A_1 v$. Brezis and Strauss [37] showed that the operator A_1 has the following properties:

Proposition 4.1. [37] *The linear operator A_1 is the $L^1(G)$ -closure of the restriction $\mathcal{A} : H_0^1(G) \rightarrow L^2(G) \subset H_0^1(G)'$ and it satisfies*

(A) *$\text{Dom}(A_1)$ is dense in $L^1(G)$ and $(I + \lambda A_1)^{-1}$ is a contraction for each $\lambda > 0$.*

- (B) $\text{Dom}(A_1) \subset W_0^{1,p}(G)$ for any p : $1 \leq p < N/(N-1)$ and there is a $c(p) > 0$ such that $c(p)\|v\|_{W_0^{1,p}} \leq \|A_1(v)\|_{L^1}$ for $v \in \text{Dom}(A_1)$.
- (C) $\sup_G (I + \lambda A_1)^{-1} f \leq \max\{0, \sup_G f\}$ for each $f \in L^1(G)$.

These properties of operator A_1 are used in [37] to study the stationary problem of structure similar to (21). In fact, remarks in [37] cover the x -dependent case but require

$$(25) \quad \text{measurability of the resolvents } (I + \bar{\beta}(x, \cdot))^{-1}$$

which is cumbersome to verify for our problem (14).

In what follows we will use (A), (C), and (B) for $p = 1$ of Proposition 4.1, and handle the x -dependence of $\bar{\beta}$ differently than in [37].

4.2. The Stationary Problem. We will show now that the proof from [37] concerning the stationary problem (21) for the case of a single maximal monotone $\bar{\beta}(\xi) = \partial\varphi(\xi)$ and an abstract operator A extends to the x -dependent case without (25) but under some additional assumptions which place the measurability hypotheses directly on the $\varphi(x, \xi)$ instead of on the resolvent. This facilitates checking the hypotheses and allows the application of the result to (14). We also prove an estimate of maximum principle type which is useful later in the analysis of the evolution problem. The maximum estimate obtained below bounds not only the values of u but also those of χ . The results are put together in Theorem 4.3 and its corollaries below.

We start by providing the construction of $\bar{\beta}$ as a subgradient of $\varphi(x, \cdot)$. For our purposes, $\varphi(x, \cdot)$ has the domain \mathbb{R} for each $x \in G$.

Definition 4.2. Assume that $\varphi(x, \xi)$ is a measurable-convex integrand with each $\varphi(x, \xi) \in [0, +\infty)$ and $\varphi(x, 0) = 0$. For each $x \in G$, denote the subgradient of $\varphi(x, \cdot)$ by

$$(26) \quad \bar{\beta}(x, \cdot) = \partial\varphi(x, \cdot).$$

Theorem 4.3. Let $\bar{\beta}(x, \cdot)$ be given as in (26). Assume additionally that

$$(27) \quad M_C(x) = \sup\{|u| : u \in \bar{\beta}(x, v), |v| \leq C\} \in L^2(G) \text{ for each } C > 0.$$

Let the linear operator $A : \text{Dom}(A) \rightarrow L^1(G)$ satisfy the following:

- (a) $\text{Dom}(A)$ is dense and $(I + \lambda A)^{-1}$ is a contraction on $L^1(G)$ for each $\lambda > 0$;
- (b) There is a $c > 0$ such that $c\|v\|_{L^1} \leq \|Av\|_{L^1}$ for $v \in \text{Dom}(A)$.
- (c) $\sup_G (I + \lambda A)^{-1} f \leq (\sup_G f)^+$ for each $f \in L^1(G)$ and $\lambda > 0$;

Then for each $f \in L^1(G)$ there is a unique solution $v \in \text{Dom}(A)$, $u \in L^1(G)$ to the stationary problem

$$(28) \quad u + Av = f \text{ and } u(x) \in \bar{\beta}(x, v(x)), \text{ a.e. } x \in G.$$

In addition, if u_1, v_1 and u_2, v_2 are solutions corresponding to f_1, f_2 , then the comparison estimates

$$(29) \quad \|(u_1 - u_2)^+\|_{L^1} \leq \|(f_1 - f_2)^+\|_{L^1}, \quad \|(u_1 - u_2)^-\|_{L^1} \leq \|(f_1 - f_2)^-\|_{L^1},$$

hold, and, consequently

$$(30) \quad \|u_1 - u_2\|_{L^1} \leq \|f_1 - f_2\|_{L^1},$$

i.e., the map $f \mapsto u$ is a contraction on $L^1(G)$.

The proof of this Theorem follows a sequence of steps. First, we recall the following result from [37] which provides key estimates there and below. Such a result holds only for a single convex function.

Lemma 4.4. ([37], Lemma 2; Prop. II.9.3 in [20]). *Let the operator A satisfy the conditions (a), (c) in Theorem 4.3, and assume the function $\varphi : \mathbb{R} \rightarrow [0, +\infty]$ is proper, convex and lower semicontinuous with $\varphi(0) = 0$. Then for each pair $v \in L^p(G)$, $u \in L^{p'}(G)$, $Av \in L^p(G)$, and $u(x) \in \partial\varphi(v(x))$ a.e. $x \in G$, with $p \geq 1$, we have*

$$\int_G Av(x)u(x) dx \geq 0.$$

For an x -dependent family of such functions, we begin with the following elementary but useful observation.

Lemma 4.5. *Assume that $\varphi(x, \xi)$ is a measurable-convex integrand with each $\varphi(x, \xi) \in [0, +\infty]$ and $\varphi(x, 0) = 0$. If $w : G \rightarrow [0, +\infty]$ is measurable, then $\varphi(x, w(x))$ is measurable. If $p \geq 1$, $v \in L^p(G)$, $u \in L^{p'}(G)$, and $u(x) \in \partial\varphi(x, v(x))$ a.e. $x \in G$, then $\varphi(\cdot, v(\cdot)) \in L^1(G)$.*

Proof. If w is measurable then from the definition (2) it follows that each Moreau-Yosida approximation $x \mapsto \varphi_\lambda(x, w(x))$ is measurable, and these converge monotonically to $\varphi(x, w(x))$ as $\lambda \rightarrow 0$, so $x \mapsto \varphi(x, w(x))$ is measurable. With u, v as indicated, we have $u(x)(0 - v(x)) \leq \varphi(x, 0) - \varphi(x, v(x))$, and this implies the integrable upper bound in $0 \leq \varphi(x, v(x)) \leq u(x)v(x)$. \square

Proof of Theorem 4.3. We follow the structure of the proof of Theorem 1 of [37]. (The latter is Theorem II.9.2 of [20]). Each step is verified for the new hypotheses.

Uniqueness of a solution is obtained from the estimate (30) and the injectivity of A . To verify (29), let u_1, v_1 and u_2, v_2 be solutions of (28) corresponding to f_1, f_2 . Subtract these two equations and multiply by $\sigma = \text{sgn}_0^+(u_1 - u_2 + v_1 - v_2)$. Since $\sigma \in \text{sgn}^+(v_1 - v_2)$ (and sgn^+ does not depend on $x \in G$), we can apply Lemma 4.4 to get $\int_G A(v_1 - v_2)\sigma dx \geq 0$. Also we have $\sigma \in \text{sgn}^+(u_1 - u_2)$, so the first of the estimates (29) follows. The second is obtained similarly by using sgn^- . These imply (30) and as in [37] that the range of $A + \bar{\beta}(\cdot)$ is closed.

To prove the existence of an approximate solution of (28), let $\epsilon > 0$ and $f_\epsilon \in L^1(G) \cap L^\infty(G)$ be fixed. (The general case $f \in L^1(G)$ follows later). For each $\lambda > 0$ consider the approximating equation

$$(31) \quad \epsilon v_\lambda + Av_\lambda + \bar{\beta}_\lambda(\cdot, v_\lambda) = f_\epsilon,$$

where we have regularized A by addition of ϵI . This is equivalent to

$$(32) \quad v_\lambda = (1 + \lambda\epsilon)^{-1}(I + \frac{\lambda}{1+\lambda\epsilon}A)^{-1}(\lambda f_\epsilon + (I + \lambda\bar{\beta})^{-1}v_\lambda).$$

The right side of (32) is a strict contraction in $L^1 \cap L^\infty$, because it is a composition of two contractions followed by scaling by a number $(1 + \lambda\epsilon)^{-1} < 1$.

Thus (32) has a unique fixed point, v_λ , a solution of (31) which depends on $\epsilon > 0$, $\lambda > 0$. Use Lemma 4.4 to test (31) with $w = \text{sgn}_0(v_\lambda) \in \text{sgn}(\bar{\beta}_\lambda(\cdot, v_\lambda))$ to obtain

$$\epsilon \|v_\lambda\|_{L^1} + \|\bar{\beta}_\lambda(\cdot, v_\lambda)\|_{L^1} \leq \|f_\epsilon\|_{L^1}.$$

Note that the function $\text{sgn}_0(\cdot)$ used to construct the test function above is independent of x , so we can use Lemma 4.4. Moreover, in the norm $\|\cdot\|$ of $L^1 \cap L^\infty$, we have from (32) that

$$\|v_\lambda\| \leq (1 + \lambda\epsilon)^{-1}(\lambda \|f_\epsilon\| + \|v_\lambda\|),$$

which implies $\|v_\lambda\| \leq \frac{1}{\epsilon} \|f_\epsilon\|$.

It remains to obtain estimates on $\bar{\beta}_\lambda(\cdot, v_\lambda)$. From (27) and the preceding estimate, $|v_\lambda(x)| \leq C$ for $C = \frac{1}{\epsilon} \|f_\epsilon\|$, so we get

$$(33) \quad |\bar{\beta}_\lambda(x, v_\lambda(x))| \leq M_C(x), \quad x \in G.$$

Hence, the sequence $\{\bar{\beta}_\lambda(\cdot, v_\lambda)\}$ is bounded in $L^2(G)$, and we follow steps identical to those in [37]. First we obtain limits $v_\lambda \rightarrow v_\epsilon$, $\bar{\beta}_\lambda(\cdot, v_\lambda) \rightarrow u_\epsilon$ as $\lambda \rightarrow 0$. Note here that we have strong limits in $L^2(G)$ due to the result from [38]. These limits satisfy

$$(34) \quad \epsilon v_\epsilon + A v_\epsilon + u_\epsilon = f_\epsilon, \quad u_\epsilon \in \bar{\beta}(\cdot, v_\epsilon).$$

Finally, for a general $f \in L^1(G)$, we approximate it with a sequence in $L^1 \cap L^\infty$, $f_\epsilon \rightarrow f$ in $L^1(G)$, solve (34) for each $\epsilon > 0$, and then we let $\epsilon \rightarrow 0$ to get $v_\epsilon \rightarrow v$ and $u_\epsilon \rightarrow u$ in $L^1(G)$ which satisfy (28). \square

Next we prove crucial comparison and maximum estimates.

Corollary 4.6. *If u_1, v_1 and u_2, v_2 are solutions corresponding to f_1, f_2 and $f_2 \geq f_1$, then $u_2 \geq u_1$ and $v_2 \geq v_1$.*

The first inequality follows from (29). The second holds for the respective approximations by (34), and hence for their limits.

Proposition 4.7. *If $f \in L^1(G) \cap L^\infty(G)$ and $k_1 \leq 0 \leq k_2$, then for any measurable selections $b_1(x) \in \bar{\beta}(x, k_1)$, $b_2(x) \in \bar{\beta}(x, k_2)$ the solution v_ϵ, u_ϵ of (34) satisfies the estimates*

$$(35a) \quad \epsilon \|(v_\epsilon - k_2)^+\|_{L^1} + \|(u_\epsilon - b_2)^+\|_{L^1} \leq \|(f - b_2)^+\|_{L^1},$$

$$(35b) \quad \epsilon \|(k_1 - v_\epsilon)^+\|_{L^1} + \|(b_1 - u_\epsilon)^+\|_{L^1} \leq \|(b_1 - f)^+\|_{L^1}.$$

Proof. Let $k_2 \geq 0$ and subtract ϵk_2 from the left side and b_2 from both sides of (34) to get

$$\epsilon(v_\epsilon - k_2) + A v_\epsilon + u_\epsilon - b_2 \leq f - b_2.$$

(Note that (27) implies $b_2 \in L^2(G)$.) Multiply by the non-negative $w(x) = \text{sgn}_0^+(v_\epsilon(x) - k_2 + u_\epsilon(x) - b_2(x)) \in \text{sgn}^+(v_\epsilon(x) - k_2) \cap \text{sgn}^+(u_\epsilon(x) - b_2(x))$ to obtain

$$\epsilon(v_\epsilon(x) - k_2)^+ + A v_\epsilon(x) w(x) + (u_\epsilon(x) - b_2(x))^+ \leq (f(x) - b_2(x))^+$$

and use Lemma 4.4 to integrate and get the first estimate. The second is proved similarly. \square

Corollary 4.8 (Maximum estimate). *In the situation of Theorem 4.3 with $f \in L^1(G)$, assume $0 \leq k$ and that $b(x) \in \bar{\beta}(x, k)$ is a corresponding measurable selection.*

If $f(x) \leq b(x)$ a.e. in G , then $v(x) \leq k$ and $u(x) \leq b(x)$ a.e. in G .

Proof. Choose the approximations f_ϵ to satisfy the same constraint as f . Then Proposition 4.7 shows the approximating solutions v_ϵ, u_ϵ of (34) satisfy the desired estimates, and the same then holds for their L^1 -limits, v and u . \square

Remark 4.2. *Corollary 4.8 does not follow from the comparison principle 4.6, since $k, b(x)$ do not need to be solutions of the boundary-value problem. When $\bar{\beta}$ is independent of x , the selection $b(x)$ can be replaced by any constant of appropriate sign to obtain L^∞ -estimates. For example, if $b \in \text{Rg}(\bar{\beta})$ we choose $k \in \mathbb{R}$ with $b \in \bar{\beta}(k)$, while for $b > \text{Rg}(\bar{\beta})$ the result is vacuously true.*

4.3. The Evolution Equation. Now we consider the evolution partial differential equation (14) with homogeneous Dirichlet boundary conditions. A solution of (14) written in terms of $u(x, t) \in \bar{\beta}(x, \chi(x, t))$ satisfies

$$(36) \quad \frac{\partial u}{\partial t} + A \circ \bar{\beta}^{-1}(\cdot, u) \ni F, \quad 0 < t < T,$$

with the operator A and monotone graphs $\bar{\beta}(x, \cdot)$ as defined in Section 4.2. We recall again the modification $\beta \rightarrow \bar{\beta}$ needed for theory, and that a general operator A or the particular operator A_1 can be used. In the latter case, (36) corresponds to (14) with the maximal monotone extension $\bar{\beta}$ of β .

Now (36) can be written as the abstract Cauchy problem (3) provided we identify \mathbb{A} and demonstrate its properties required by Theorem 2.4.

The extended Brezis-Strauss Theorem 4.3 developed in Section 4.2 provides the construction of the appropriate operator

$$(37) \quad \mathbb{A} = A \circ \bar{\beta}^{-1}(\cdot, \cdot)$$

in $L^1(G)$. Define the relation \mathbb{A} on $L^1(G)$ by $\mathbb{A}(u) \ni f$ if $u \in L^1(G)$, $f \in L^1(G)$ and that for some $\chi \in \text{Dom}(A)$,

$$A\chi = f \text{ and } u(x) \in \bar{\beta}(x, \chi(x)), \text{ a.e. } x \in G.$$

The Cauchy problem (3) with this operator \mathbb{A} is equivalent to the abstract problem which can be rewritten as

$$(38) \quad u'(t) + A\chi(t) = F(t), \quad u(t) \in \bar{\beta}(\cdot, \chi(t)), \quad 0 < t < T, \quad u(0) = u_0.$$

To show \mathbb{A} is m-accretive, we use results of Section 4.2. The equation (28) is equivalent to $u + \mathbb{A}(u) \ni f$, and Theorem 4.3 implies that the map $f \mapsto u$ is a contraction defined on $L^1(G)$. Moreover, the same holds with A replaced by λA for any $\lambda > 0$, so \mathbb{A} is m-accretive in the Banach space $L^1(G)$. Thus Theorem 2.4 applies, and we have the following result.

Proposition 4.9. *In the situation of Theorem 4.3, the corresponding initial-value problem (38) is well-posed. That is, for each $u_0 \in \overline{\text{Dom}(\mathbb{A})}$ and $F(\cdot) \in L^1(0, T; L^1(G))$ there is a unique C^0 solution of (36) with $u(0) = u_0$.*

We continue now to derive estimates on the solution to (36) which help to determine whether the a-priori extension $\beta \rightarrow \bar{\beta}$ limits the applicability of Proposition 4.9, namely, whether the solution of (36) satisfies (14). This is the case if we can show that the solution satisfies (15).

Corollary 4.10 (Comparison principle). *If $u_1(t), v_1(t)$ and $u_2(t), v_2(t)$ are solutions of the initial-value problem (38), with the corresponding data $u_1(0), F_1(t)$ and $u_2(0), F_2(t)$, then*

$$\begin{aligned} \|(u_1(t) - u_2(t))^+\|_{L^1} &\leq \|(u_1(0) - u_2(0))^+\|_{L^1} \\ &+ \int_0^t \|(F_1(s) - F_2(s))^+\|_{L^1} ds, \quad 0 \leq t \leq T, \end{aligned}$$

and similar inequalities hold for $\|(u_1(t) - u_2(t))^-\|_{L^1}$ and $\|u_1(t) - u_2(t)\|_{L^1}$.

Proof. This follows immediately for the approximations (5) by the estimates (29). \square

Corollary 4.10 and Corollary 4.8 yield bounds on a solution as follows.

Remark 4.3. *Let*

$$(39a) \quad v_2 \in \text{Dom}(A) \text{ with } Av_2 = F_2 \geq 0, \text{ and}$$

$$(39b) \quad u_0(x) \leq u_2(x) \in \bar{\beta}(x, v_2(x)) \text{ in } L^1(G).$$

From Corollary 4.10 we find that if $F \leq 0$, then the solution of (38) satisfies

$$(40) \quad u(t) \leq u_2, \quad \chi(t) \leq v_2, \quad 0 \leq t \leq T.$$

We also find that if $F \equiv 0$, then

$$(41) \quad u_0 \geq 0 \implies u(t) \geq 0.$$

Similarly, we obtain a *maximum estimate* for the initial-value problem for $\mathbb{A} = A \circ \bar{\beta}^{-1}(\cdot, \cdot)$.

Corollary 4.11 (Maximum estimate). *If $F \leq 0$, and*

$$(42a) \quad 0 \leq k, b(x) \in \bar{\beta}(x, k)$$

is a measurable selection, and

$$(42b) \quad u_0(x) \leq b(x) \text{ a.e.,}$$

then the C^0 -solution of the Cauchy problem (38) satisfies

$$(43) \quad u(x, t) \leq b(x), \quad \chi(x, t) \leq k, \text{ a.e. } x \in G,$$

for $0 \leq t \leq T$.

Proof. This follows immediately for the approximations (5) by the estimates of Corollary 4.8. \square

It follows from Corollary 4.11 that the solution of (38) is completely independent of those values of $u \in \bar{\beta}(x, \chi)$ with $u \geq b$ or $\chi \geq k$. In other words, we can extend $\beta(x, \cdot)$ to a maximal monotone graph $\bar{\bar{\beta}}(x, \cdot)$ in any (monotone) way for $u \geq b, \chi \geq k$.

Remark 4.4. *If the initial data for the problem (14) can be shown to satisfy (42) for some useful pair $k, b(x)$, then the solution to (36) remains bounded by the same pair. Thus it does not matter how the graph β was extended to $\bar{\beta}$ beyond k, b . We can conclude the well-posedness for the problem (14) with the original $\beta(x, \cdot)$ for the initial data satisfying (42).*

The remaining difficulty is to identify whether we can find useful bounds b, k which correspond to physically meaningful solutions, in particular those that yield solutions that satisfy (15). Examples shown in Section 5 address this question.

4.4. Handling nonconstant ϕ and nonhomogeneous boundary conditions. The analysis given above was formulated for homogeneous boundary conditions and for constant porosity coefficient set as in (12).

Remark 4.5. *One can treat nonconstant porosity coefficient as follows. If $\phi \in L^\infty(G)$ and $\phi(x) > 0$ for a.e. $x \in G$, then $u \in \partial\varphi(x, v)$ is equivalent to $\phi(x)u \in \partial(\phi(x)\varphi(x, v))$ for $x \in G$, and the functions $\phi(x)\varphi(x, v)$ and $\phi(x)\beta(x, v)$ have the same respective properties as $\varphi(x, v)$ and $\beta(x, v) = \partial\varphi(x, v)$.*

The case of $\phi(x, t)$ is important e.g., since ϕ depends on the pressure, but is considerably more difficult from analysis point of view and will not be discussed here.

Next, we discuss boundary conditions. For linear smooth problems the extension of analysis to non-homogeneous Dirichlet conditions (needed in applications) is straightforward. For (14) this is also true, but shifting of boundary conditions affects various maximum and comparison principles. We address the case of nonhomogeneous boundary conditions in detail for completeness, and do not revisit analyses formulated above.

Suppose we want to resolve the evolution equation

$$(44) \quad \frac{d}{dt}u(t) + A_1v(t) = F(t), \quad u(t) \in \bar{\beta}(\cdot, v(t)),$$

in $L^1(G)$ with given initial value $u(0)$, where A_1 is the partial differential operator above but with non-homogeneous boundary conditions on $v(t)$, independent of t . Let $v_0 \in W^{2,1}(G)$ be a smooth function that satisfies those boundary conditions, that is, v and v_0 have the same trace on ∂G and $A_1v_0 \in L^1(G)$. Choose $u_0 \in L^1(G)$ to satisfy $u_0(x) \in \bar{\beta}(x, v_0(x))$ for $x \in G$. Then define the translates

$$\begin{aligned} \tilde{\beta}(x, \xi) &= \bar{\beta}(x, v_0(x) + \xi) - u_0(x), \quad \xi \in \mathbb{R}, \\ \tilde{u}(t) &= u(t) - u_0, \quad \tilde{v}(t) = v(t) - v_0, \quad \tilde{F}(t) = F(t) - A_1v_0 \end{aligned}$$

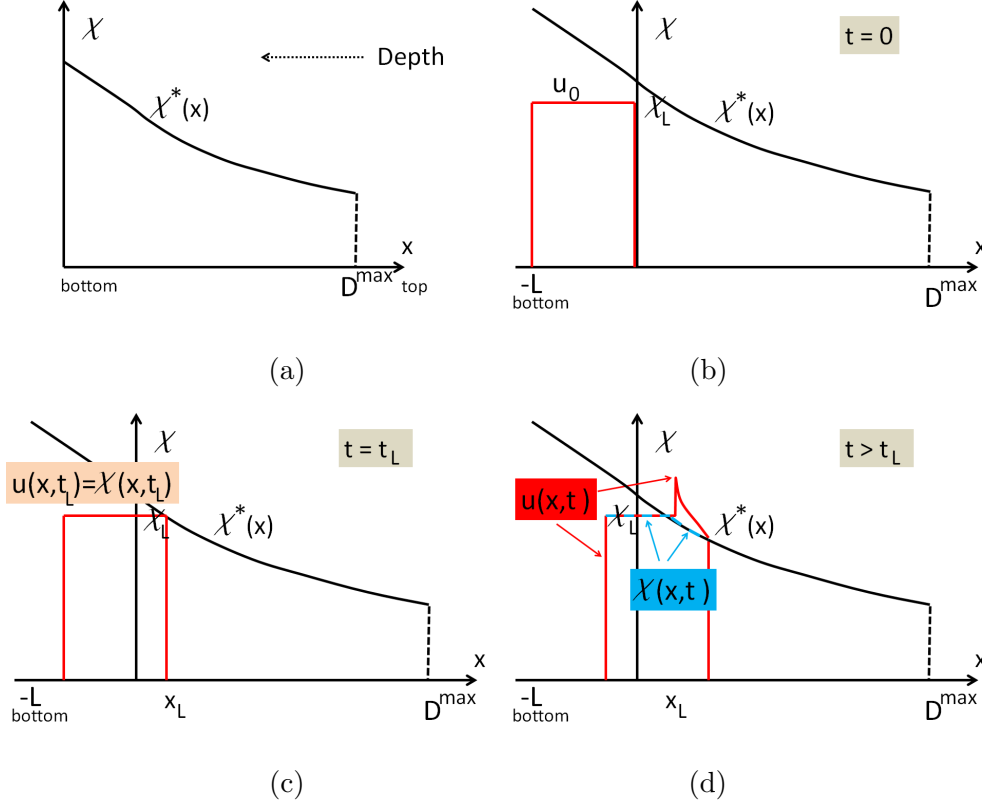


FIGURE 1. (a) Example of χ^* for a typical reservoir as in [6]. (b)-(d) Example in Section 5.2 at $t = 0$, $t = t_L$, and $t > t_L$, respectively.

Each $\tilde{\beta}(x, \cdot)$ is maximal monotone, $\tilde{\beta}(x, 0) = \tilde{\beta}(x, v_0(x)) - u_0(x) \ni 0$, $\tilde{v} = 0$ on ∂G , and

$$(45) \quad \frac{d}{dt} \tilde{u}(t) + A_1 \tilde{v}(t) = \tilde{F}(t), \quad \tilde{u}(t) \in \tilde{\beta}(\cdot, \tilde{v}(t)).$$

Conversely, if $\tilde{u}(t), \tilde{v}(t)$ is a solution of (45) with $\tilde{v}(t) \in \text{Dom}(A_1)$, then $u(t), v(t)$ is a solution of (44) with the prescribed boundary values $v(t)|_{\partial G} = v_0|_{\partial G}$.

To apply this observation to get estimates on solutions of (44) from those we have on the equation (45) with homogeneous boundary conditions, it is useful to note that we can always choose v_0 to have the same upper or lower bounds as its trace on the boundary. For example, we could choose v_0 to be a harmonic function with the prescribed boundary values.

5. EXAMPLES OF WHERE THEORY APPLIES AND WHERE IT DOES NOT

In this Section we illustrate the well-posedness results from Section 4 and their limitations. In particular, we exhibit explicit examples and applications of the maximum and comparison principles. This is the task that was outlined after Remarks 4.3 and 4.4. The goal is to use the comparison and maximum principles to verify (15). This may be possible by putting appropriate restrictions on the data for some cases, and then the extension $\beta \rightarrow \tilde{\beta}$ does not change the problem, and we have full well-posedness in those cases, with solutions satisfying physically meaningful bounds (15).

We first discuss the applications of maximum and comparison principles and then consider an analytical solution to a simplified case of (14) with pure advection in $N = 1$. Such a scenario arises when the system changes rapidly away from hydrostatic equilibrium and when diffusion

is negligible compared to advection. It also presents the “worst case scenario” from the point of view of analysis while it simultaneously accounts for the largest possible accumulation of hydrate. The scenario leads to hydrate saturations exceeding 1 which is unphysical and can be considered a “blow-up”. We discuss whether this blow-up can be anticipated or prevented by the maximum or comparison estimates.

In all of the examples below we assume

$$(46) \quad \chi^*(x) \text{ is a smooth non-increasing function in } G,$$

which is consistent with typical phase behavior in subsea sediments [6]; see Figure 1(a). For simplicity we consider $N = 1$ and that the reservoir

$$(47) \quad G := (0, D^{max})$$

has its bottom at $x = 0$ and its top $x = D^{max}$ near the seafloor. We also assume constant porosity (12) and homogeneous boundary conditions.

5.1. Application of maximum and comparison principles. We consider two main examples of purely diffusive and purely advective transport. Both are included in the theory.

We have two tools to obtain estimates on a solution of the stationary problem (28) which result eventually in those for the evolution problem (36). The first is the comparison principle (29) of Theorem 4.3 which bounds one solution by another solution. The difficulty here is to choose solutions which provide useful estimates. The second tool follows the maximum estimate in Corollary 4.8 which provides bounds which are not solutions. If β is independent of x , the constants are arbitrary, but in the x -dependent case the bound is a function chosen from the level set of $\beta^{-1}(x, \cdot)$.

5.1.1. Purely diffusive case. Let $D_l^M > 0$, $q = 0$.

The well-posedness result of Proposition 4.9 applies to the operator $A = -D_l^M \frac{d^2}{dx^2}$ with domain

$$Dom(A) = \{v \in W^{2,1}(G) : v(0) = v(D^{max}) = 0\},$$

and one can see that it satisfies the hypotheses of the Theorem 4.3 on $L^1(G)$. Thus there is a unique C^0 solution to the problem (38).

We would like to use Remark 4.3 with $v_2 = \chi^*$, but the assumption (39) requires that $\chi^* \in Dom(A)$ and $A\chi^* \geq 0$; it allows for sink terms but no sources. Consider the particular case

$$(48) \quad \text{affine, decreasing } \chi^*, \text{ initial data } u_0 \leq R,$$

with homogeneous boundary conditions, pure diffusion with sinks.

Let $\delta > 0$ and choose $v_2 \in Dom(A)$ to be concave, $0 \leq v_2 \leq \chi^*$, and $v_2(x) = \chi^*(x)$ for $x \in (\delta, D^{max} - \delta)$. Select $u_2 \in \beta(\cdot, v_2)$ by $u_2(x) = R$ for $x \in (\delta, D^{max} - \delta)$ and $u_2 = v_2$ otherwise in G . Thus, if $0 \leq u_0 \leq u_2$ and $F \leq 0$, we obtain from Remark 4.3 that $0 \leq u(t) \leq u_2 \leq R$ and $\chi(t) \leq v_2$ in G , so we have a (physical) solution to (14) that satisfies (15) for all time. Note this case was obtained independently (in $H^{-1}(G)$) in [14]. An extension of (48) is possible for a concave χ^* , which is, however, a nonphysical situation.

5.1.2. Purely advective case. Now consider $D_l^M = 0$, $q = const > 0$. We develop an explicit analytical solution for this case below and concentrate on the estimates first. To apply the well-posedness result of Proposition 4.9 we see that the abstract formulation includes the operator $A = q \frac{d}{dx}$ with domain

$$(49) \quad Dom(A) = \{v \in W^{1,1}(0, D^{max}) : v(0) = 0\},$$

which satisfies the hypotheses of Theorem 4.3 on $L^1(G)$. Thus there is a unique C^0 solution to the problem; it is given in Lemma 5.1 below.

Now we would like to apply the maximum estimate to give a bound $b(x) \leq R$ which would yield (15). Choose $k \geq 0$ and $b(x) \in \beta(x, k)$. Then $b(x) \leq R$ implies $k \leq \chi^*(x)$ for every $x \in (0, D^{max}]$. Thus $b(x) = k$ for all $x \in G$. But the largest possible $k = \chi^*(D^{max}) \leq \chi^*(x)$ by (46), so we obtain

$$(50) \quad S(x, t) = 0, (x, t) \in G \times (0, T).$$

Thus the problem with

$$(51) \quad \begin{aligned} &\text{non-increasing } \chi^*, \text{ initial data } u_0 \leq \chi^*(D^{max}), \\ &\text{null boundary condition at 0, only advection, and no sinks/sources,} \end{aligned}$$

is well posed with the original β . While physical, there is no hydrate formation in this example with such data.

To use the comparison principle to get an upper bound $b(x) = R$ for a more realistic example with hydrate formation, i.e., $S(x, t) > 0$ for some x, t , we would like to choose $v_2 = \chi^*$. However, $\chi^* \notin \text{Dom}(A)$ given by (49) because it does not satisfy the boundary condition. However, if we truncate it linearly so that

$$v_2(x) := \begin{cases} \chi^*(x), & x \geq x_0 > 0, \\ \chi^*(x_0) \frac{x}{x_0}, & 0 < x < x_0, \end{cases}$$

then we can choose

$$b(x) := \begin{cases} R, & x \geq x_0 > 0, \\ \chi^*(x_0) \frac{x}{x_0}, & 0 < x < x_0. \end{cases}$$

These would give a good bound except that

$$Av_2(x) = \begin{cases} q \partial_x \chi^*(x), & x \geq x_0 > 0, \\ q \chi^*(x_0), & 0 < x < x_0, \end{cases}$$

and the assumption $Av_2 \geq 0$ holds only if $q \partial_x \chi^* \geq 0$. This requires, for the flow towards the ocean floor ($q > 0$), to have χ^* to be nondecreasing, which is unphysical, a clear contradiction with (46).

Alternatively, one can have the profile as shown in Figure 1, but with flux $q < 0$ working towards the bottom of the reservoir (which requires boundary condition to be defined at $x = D^{max}$ and not at $x = 0$). In summary, this case is

$$(52) \quad \begin{aligned} &\text{decreasing } \chi^*, \text{ initial data } u_0 \leq R, \\ &\text{with null boundary condition on right, only advection, no sinks, } q < 0. \end{aligned}$$

This case is well-posed without an extension of β but is rarely seen in practice. On the other hand, the case

$$(53) \quad \begin{aligned} &\text{decreasing } \chi^*, \text{ initial data } u_0 \leq R, \\ &\text{null boundary condition on left, only advection, no sinks, } q > 0, \end{aligned}$$

requires an ad-hoc extension $\beta \rightarrow \bar{\beta}$ for well-posedness and may have unphysical solutions, since (15) cannot be guaranteed with the maximum and comparison principles derived in Section 4.

These findings are consistent with the analytical solution we derive below for the case (53) in which a “blow-up” occurs with $S > 1$ at some critical time t_* in violation of (15). However, one can still extend $\beta \rightarrow \bar{\beta}$ beyond some possible maximum value of χ^*, u which depends on the data, and have well-posedness of the problem with $\bar{\beta}$ producing solutions which are unphysical past t_* . We interpret this as a case for which we have only local in time physical solution, and simultaneously one in which the model itself becomes unphysical.

5.2. Analytical solution for advection case. We calculate the solution to (14) in the case (53) with constant flux input. We set $G = (-L, D^{max})$ for some $L > 0$ and consider

$$(54a) \quad \partial_t u + \partial_x(q\chi) = 0, \quad x \in G, \quad t > 0$$

in which $u = (1 - S)\chi + RS \in \beta(x, \chi)$ is determined by (11d). The initial condition for the problem is

$$(54b) \quad u(x, 0) = \begin{cases} \chi_L, & x \leq 0, \\ 0, & x > 0 \end{cases} = \chi_L H(-x),$$

where H is the Heaviside function. This describes the physical situation in which no methane is initially present in the reservoir $(0, D^{max})$, but as time progresses, a uniform pulse of methane of a fixed concentration and duration enters the reservoir at the left boundary and gets transported towards the right (upper) boundary into the reservoir.

Remark 5.1. *The boundary condition at $x = 0$ implicit in (54b) is inhomogeneous and thus not covered by the theory in Section 4, but it can be included by posing the problem on $(-L, D^{max})$ with $u(-L, t) = 0$ as indicated, and setting $u_0(x) = \chi_L H(-x)$.*

We assume that $\chi_L < \chi^*(0)$, i.e., the incoming methane is all dissolved in the water. There is no outflow boundary condition on the right end for this first order equation (54).

Lemma 5.1. *Assume*

$$(55) \quad \chi^*(0) > \chi_L \geq \min\{\chi^*(x) : x \in G\}.$$

Let x_L be the unique last point where

$$(56) \quad \chi_L = \chi^*(x_L),$$

and define the zones

$$(57a) \quad G_-(t) \equiv \{x : 0 < x < \min(qt, x_L)\},$$

$$(57b) \quad G_0(t) \equiv \{x : x_L < x < qt\},$$

$$(57c) \quad G_+(t) \equiv \{x : x > qt\}.$$

Then the solution $\chi(x, t), S(x, t)$ to (54) is given by

$$(58a) \quad \chi(x, t) = \min(\chi_L, \chi^*(x))H(qt - x),$$

$$(58b) \quad S(x, t) = -\frac{(t - t_x)^+ q \partial_x \chi^*(x)}{R - \chi^*(x)}, \quad x \in G_0(t),$$

$$(58c) \quad S(x, t) = 0, \quad x \in G_-(t) \cup G_+(t),$$

where $t_x \equiv \frac{x}{q}$ is the breakthrough time for each position x , that is, the first time at which methane is present at x .

Proof. As time t increases, the methane enters the reservoir and much of it is transported upwards towards the ocean floor located at $x = D^{max}$ and escapes there. However, some of the methane remains trapped in the reservoir in the form of hydrate because of (55). Since χ^* is monotone decreasing, there is a unique last point $x_L \in \bar{G}$ for which (56) holds. The methane which enters G from the left travels up to x_L as a travelling wave $\chi(x, t) = \chi_L H(qt - x)$, $0 < x < x_L$, with speed q . The dissolved amount $\chi(x, t)$ does not exceed $\chi^*(x)$, $x \leq x_L$, thus we have $S(x, t) = 0$, $u(x, t) = \chi(x, t)$, $0 < x < x_L$.

In summary, for $tq \geq x$ or $t \geq t_x$, we have $\chi(x, t) = \min(\chi_L, \chi^*(x))$ and there is no methane $u(x, t) = \chi(x, t) = 0$ ahead of the travelling wave where $tq < x$ ($t < t_x$). This is concisely written as (58a).

One can thus distinguish three zones (57). Note that $G_-(t)$ and $G_0(t)$ are empty for $qt < x_L$. While the right boundaries of G_- and G_0 travel with speed q , the left boundary x_L of G_0 is a *free boundary* determined by the solution.

Now $u(x, t)$ must be partitioned between the flowing dissolved methane advected towards the right and the stationary hydrate phase in G_0 with saturation S . Furthermore, $u(x, t)$ increases due to the continuous supply of gas advected from the left. We have by (13) and (58a) that

$$(59) \quad u(x, t) = (1 - S)\chi^*(x)H(qt - x) + RS, \quad x > x_L,$$

and we can formally differentiate in time to get

$$(60) \quad \partial_t u = \partial_t S(x, t)(R - \chi^*(x)H(qt - x)) + (1 - S)\chi^*(x)q\delta(qt - x).$$

Here we have used Dirac δ for $\partial_t H$. Differentiating (58a) in x we have

$$\partial_x \chi = \partial_x \chi^*(x)H(qt - x) - \chi^*(x)\delta(qt - x).$$

Since $S(x, t)\delta(qt - x) = 0$, substituting these into the conservation law (54a) yields

$$(61) \quad S_t(R - \chi^*(x)H(qt - x)) + q\partial_x \chi^*(x)H(qt - x) = 0, \quad x > x_L.$$

In $G_- \cup G_+$ clearly $S \equiv 0$ and $S_t = 0$ since these regions are undersaturated.

It remains to calculate $S(x, t), x \in G_0(t)$. From (61) we have

$$S_t = -\frac{q\partial_x \chi^*(x)}{(R - \chi^*(x))}, \quad x \in G_0(t),$$

and integrating in time from t_x to t , with $S(x, t_x) = 0$ gives (58b). □

Remark 5.2. *Another way to calculate (58b) is to notice that*

$$(62) \quad \partial_t u = -q\partial_x \chi^*(x), \quad x \in G_0(t),$$

which is exactly (54a) written in $G_0(t)$. Integrating the right hand side in time we have

$$(63) \quad u(x, t) - u(x, t_x) = -(t - t_x)q\partial_x \chi^*(x), \quad x \in G_0(t)$$

With (13) we now see

$$(64) \quad (1 - S(x, t))\chi^*(x) + RS(x, t) - (1 - S(x, t_x))\chi^*(x) + RS(x, t_x) \\ = -(t - t_x)q\partial_x \chi^*(x), \quad x \in G_0(t).$$

However, $S(x, t_x) = 0$ thus we further simplify to obtain

$$(65) \quad S(x, t)(\chi^*(x) - R) = (t - t_x)q\partial_x \chi^*(x), \quad x \in G_0(t).$$

which is the same as (61).

From these, it follows that if the pulse of methane is not too large, i.e.,

$$(66) \quad \frac{L(-\partial_x \chi^*(x))}{R - \chi^*(x)} \leq S_0 < 1, \quad x \geq x_L,$$

then $S(x, t) < 1$ and the constraint (15) is satisfied.

Otherwise, from (61) we see that S reaches 1 at $t = t_*$ given by

$$(67) \quad t_* = t_x + \frac{\chi^*(x) - R}{q\partial_x \chi^*(x)}.$$

This time can be calculated for a given χ^* with known R and q . Note that by (11b), (13), $q > 0$, (46), we have $t_* > t_x$.

At $t > t_*$, we have that $S > 1$, i.e., (15) is violated. We have thus demonstrated an important observation which we shall discuss in view of the maximum principles discussed earlier.

Corollary 5.2. *The solution satisfies (15) if (66) holds. Otherwise, there is no physically meaningful solution to (54) for $t > t_*$ where t_* is given by (67).*

6. THE COUPLED TRANSPORT-PRESSURE SYSTEM

Now we discuss the system consisting of the transport (saturation) equation (14) solved for methane solubility χ , and methane content u . In what follows we assume that all variables can be defined pointwise at every x . (More formally, we use their regularizations as described below). We also assume that there is nontrivial diffusion present in the problem, so elliptic regularity applies.

We recall that from (13) we have

$$(68) \quad S = \frac{(u - \chi^*)^+}{R - \chi^*},$$

that is, S is a Lipschitz function of u . (Obviously, (68) is true at every $x \in G, t > 0$).

The transport model (14) is coupled with the time-independent pressure equation (17) solved for p and \mathbf{q} . The system (14) and (17) is fully coupled because the permeability $\kappa(x, S(x, t))$ varies with the hydrate saturation. One could consider the more general pressure equation (16), but this will not be done here.

The pressure equation (17) is elliptic in p and is easily resolved at any fixed time. Since κ varies with S , it varies with time, thus so do $p = p(t)$ and $\mathbf{q} = \mathbf{q}(t)$. But the linear operator A in the abstract formulation of the transport equation contains \mathbf{q} and thus is time dependent. As such, the coupled case is not covered directly by the theory developed in Section 4.

We consider therefore a time-staggered coupling in the system, which allows the treatment of transport and pressure components separately.

Let $0 = t_0 < t_1 < \dots t_n < \dots t_N = T$ be a sequence of discrete time intervals. Let $u_0 = u(t_0) \in \text{Dom}(A)$.

For $n = 0, 1, 2, \dots$ we proceed as follows.

- (1) For each n , given $u(t_n)$, we can calculate $S(u(t_n))$ using (68). Then we can calculate $\kappa(t_n) = \kappa(S(u(t_n)))$ from (20). Next we solve the quasi-static pressure equation (17) for $\mathbf{q}(t_n)$.
- (2) Given $u(t_n)$, $\mathbf{q}(t_n)$ we solve (14) for $u(t) \in \beta(x, \chi(t))$, $t_n \leq t \leq t_{n+1}$.
- (3) Return to step (1) with n replaced by $n + 1$.

This procedure depends on the exchange of data between (14) and (17). However the solution of the saturation equation (14) is rather weak, and we only have $u(t) \in L^1(G)$ and $\chi(t) \in \text{Dom}(A_1)$. We alter (2) by regularizing (14) with the Lipschitz β_λ and $A_\epsilon = A + \epsilon I$, as in the proofs of Section 4, so the corresponding solutions $u_{\lambda, \epsilon}$ are good approximations of the solution u of (14) when ϵ and λ are small.

Since $S(u_{\lambda, \epsilon})$ is smooth, the coefficient $\kappa_{\lambda, \epsilon} = \kappa(S(u_{\lambda, \epsilon}))$ is also smooth. From the pressure equation (17) we know that the corresponding $\mathbf{q}_{\lambda, \epsilon} \in H_{div}^1(G)$, but it will be smoother for the approximating equation. Typically, we can appeal to classical regularity results [21, 39] to see that if $\kappa_{\lambda, \epsilon} \in C^{0, \gamma}(G)$ with $0 < \gamma < 1$, then the solution of the elliptic equation (17) satisfies $p_{\lambda, \epsilon}(t) \in W^{2, s}(G) \cap C^{1, \gamma}(G)$ for some $s \geq 1$, so the flux $\mathbf{q}_{\lambda, \epsilon}(t) \in H^{1, s}(G) \cap C^{0, \gamma}(G)$. (Of course, in the $N = 1$ case, the flux is constant and determined by boundary conditions.)

Conversely, given $q_{\lambda, \epsilon}(t_n)$ we want to see if it is smooth enough to construct $A(t_n)$ and solve (14) and close the loop, so that the exchange of data in the iterative coupling is meaningful. For $N = 1$ it is obviously true. For $N > 1$ we only have $\mathbf{q}_{\lambda, \epsilon}(t_n) \in C^{0, \gamma}(G)$, $\gamma < 1$ which falls somewhat short of the formally required condition $\mathbf{q}(t_n) \in C^1(G)$. However, this shortcoming can be avoided by additional minor regularization.

It is understood that $\kappa \geq \kappa_0 > 0$ in G . If this is violated, then $\mathbf{q} \rightarrow \mathbf{0}$ and a geomechanics component is required for the model.

7. CONCLUSIONS

In this paper we have extended previous work [14] on a diffusive model of methane transport with hydrate formation to the case which includes advective transport coupled to an appropriate pressure equation. The well-posedness of the model is formulated in Proposition 4.9 along with some comparison and maximum principles that work for various practical cases. However, for other cases, an extension of data required for well-posedness may produce unphysical solutions, where hydrate saturation (volume fraction) exceeds one.

This result was apparent from both the maximum and comparison principles that we constructed, as well as from an analytical solution to an initial-boundary-value problem that we constructed for the purely advective case in $N = 1$. Thus there arise the questions of the relevance of the analysis and the range of application of model.

In fact, it is the oversimplifications of the model that lead to the unphysical case where (15) is violated. When the entire pore space is clogged by hydrate, as when $S = 1$, the fluid ceases to flow, thus $q = 0$. Since a one-dimensional model does not allow it, it is therefore producing unphysical solutions. Even before $S = 1$, the model coupled to the pressure equation must account for the decrease of $\kappa = \kappa(x, S, p(x))$, thus increased pressure and fracturing. Eventually, the transport and pressure equation model should be extended to include a mechanics component with deformation or fracturing. This is a subject of ongoing work.

Other extensions currently underway include accounting for nonconstant salinity χ_l^S , and temperature, and for more general thermodynamics such as that for when water is not available for hydrate formation.

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